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Calculating Shuffler Count Rates

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by

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ABSTRACT

Shufflers measure fissile masses nondestructively by counting delayed neutrons released after successive irradiations from ^{252}Cf neutrons. The count rates are best correlated to fissile masses through calibration with certified standards. But certified standards exist for only a few material types and packaging, while measurements are needed on a very wide variety of materials. A new method for calculating count rates is described in this report. It may be used for calibration without standards or for bias corrections to a calibration based on certified standards. This report is for those who want to understand and apply the process of calculating count rates.

INTRODUCTION

The method for calculating shuffler count rates uses an analog simulation of the shuffler. No shortcuts or significant approximations are used. Even the motion of the ^{252}Cf source during an irradiation is simulated.

The following codes and information are needed to perform a complete calculation.

- An accurate MCNP model of the shuffler and the items in the assay chamber.
- MCNP and its associate cross-section libraries, all installed on a computer.
- A PC with Excel 97 (or later).
- The Excel spreadsheet "CPS1.XLS" for any number of cells each with the *same* one or more fissile material combined in a single tally, or "CPS2.XLS" for two cells with *different* fissile materials. (The macros in CPS2.XLS could easily be extended to any number of cells).
- Delayed neutron parameters (decay constants; delayed neutron yields per fission) for the fissile materials.
- The yield *Y* of the shuffler's ^{252}Cf source. (The situation where this is not well known will be discussed later.)
- The detection efficiency of delayed neutrons. (Ways to determine the efficiency will be given later.)
- The assay parameters (times, distances, number of shuffles).

Each spreadsheet shows the user where the numerical information is to be placed.

The user prepares only one MCNP input file; all the others are generated by the spreadsheet by copying that file and changing the ^{252}Cf position. Likewise, the spreadsheet reads all of the MCNP output files and extracts the fission probabilities and their uncertainties. A plot is made of these results so that a judgment can be made on their relative correctness.

Finally, the delayed neutron counts and count rates are calculated by the spreadsheet.

CALCULATION FUNDAMENTALS

The basic mathematical description of shufflers is developed in Ref. 1 where Eq. (17) gives the number of delayed neutrons *D* produced during an assay. That equation is reproduced here as Eq. (1) with a multiplication factor M_{DN} included for delayed neutrons from larger fissile masses.

$$D = M_{DN} \sum_{j=1}^{6} \left(\frac{\varepsilon \cdot f \cdot \beta_j}{\lambda_j} \right) \cdot \left(1 - e^{-\lambda_j \cdot t_i} \right) \cdot \left(e^{-\lambda_j \cdot t_r} \right) \cdot \left(1 - e^{-\lambda_j \cdot t_c} \right) \cdot \left[\frac{n - (n+1) \cdot e^{-\lambda_j \cdot \tau} + e^{-(n+1) \cdot \lambda_j \cdot \tau}}{\left(1 - e^{-\lambda_j \cdot \tau} \right)^2} \right] \quad (1)$$

The meaning of the various parameters will not be explained here; see Ref. 1 if they are unfamiliar.

This expression was developed while assuming that the fission rate f is constant. This is not correct if the source scans during irradiation, as the sources in the large 55-gallon drum shufflers generally do. However, the number of delayed neutron precursors in group *j* that exist after an irradiation is

$$P_j(t_i) = \left(\frac{f \cdot \beta_j}{\lambda_j} \right) \cdot \left(1 - e^{-\lambda_j \cdot t_i} \right). \quad (2)$$

Equation (1) can therefore be written without reference to *f*.

$$D = M_{DN} \, \varepsilon \cdot \sum_{j=1}^{6} P_j(t_i) \cdot \left(e^{-\lambda_j \cdot t_r} \right) \cdot \left(1 - e^{-\lambda_j \cdot t_c} \right) \cdot \left[\frac{n - (n+1) \cdot e^{-\lambda_j \cdot \tau} + e^{-(n+1) \cdot \lambda_j \cdot \tau}}{\left(1 - e^{-\lambda_j \cdot \tau} \right)^2} \right] \quad (3)$$

All that really matters is the number of precursors that exist after the irradiation, not whether the irradiating neutron flux from the ^{252}Cf source was constant or not. To use Eq. (3) we need to calculate $P_j(t_i)$ for a single irradiation; the effect of repeating this for *n* shuffles is accounted for by Eq. (3).

The evaluation of $P_j(t_i)$ is done by numerically solving the basic equation for the population of delayed neutron precursors (see Ref. 1).

$$\frac{dP_j}{dt} = f(t) \cdot \beta_j - \lambda_j \cdot P_j(t) \quad (4)$$

Notice that *f* is written as a function of time here. It is closely related to the probability of a neutron from ^{252}Cf inducing a fission in the fissile material.

$$f(t) = p_{fission}(t) \cdot Y \cdot \bar{\upsilon} \quad (5)$$

Y is the neutron yield (neutrons per second) from the ^{252}Cf source and $\bar{\nu}$ is the average number of fission neutrons released per fission. The fission probability $p_{fission}$ at some fixed position of the ^{252}Cf source is calculated with MCNP. A set of calculations for different positions gives a corresponding set of $p_{fission}$ values. But $p_{fission}(t)$ is not yet known.

The scanning protocol specifies where the ^{252}Cf source is as a function of time during a single irradiation period. In effect, a table is generated like Table I that gives $p_{fission}(t)$ at a set of closely spaced times ready for numerical integration applications. The values for $p_{fission}(t)$ for positions outside those used for the MCNP calculations are interpolated from those that were calculated. The time interval used in Table I is 0.001 s and this has been found to give very accurate results. Larger time intervals may be adequate, but this topic has not been thoroughly explored. This short time works well and the computation time is very short (practically instantaneous on a modern computer).

Table I. Specifying $p_{fission}(t)$: An Example

Time	^{252}Cf Distance* (in.)	Interpolated $p_{fission}(t)$
0	60	6.454E-04
0.001	60	6.454E-04
0.002	60	6.454E-04
….	….	….
1.100	58.06	7.806E-04
1.001	58.07	7.807E-04
….	….	….
2.306	55.95	8.372E-04
….	….	….

* This is the distance the source moved from the stored position. The Excel spreadsheet code needs to know how to convert this to a distance suitable for the MCNP input files.

With $p_{fission}(t)$ known in tabular form for closely space times, we also know $f(t)$ numerically from using Eq. (5). Equation (4) can now be solved numerically starting with $P_j(0) = 0$ and working up to the end of the irradiation at $t = t_i$. The simplest numerical integration technique has worked very well.

$$P_j(t+\Delta t) \approx P_j(t) + \Delta P_j(t) = P_j(t) + [\, f(t) \cdot \beta_j - \lambda_j \cdot P_j(t)] \cdot \Delta t \qquad (6)$$

The fourth-order Runge-Kutta algorithm was also implemented and tested, but the results were identical to those from Eq. (6), so the simpler procedure continues to be used.

All of these calculations, except for the MCNP runs, are done within the EXCEL "macro" called "Calculate_count_rate" that is part of "CPS1.XLS" and "CPS2.XLS." The "macro" is written using the Visual BASIC provided with Excel. After clicking on a virtual button to start the calculation, the numerical integration is performed and counts from Eq. (3) are calculated in a fraction of a second. The count rate is D/T_c, where T_c is the total count time over all the shuffles (= $n\ t_c$).

A CALCULATION'S UNCERTAINTY

The uncertainty of a calculated delayed neutron count *D* takes into account the uncertainties of the detection efficiency ε and the $p_{fission}$ values. The uncertainties of other parameters are assumed to be insignificant by comparison. The efficiency and multiplication directly affect the count and its error introduces a corresponding bias in the result. The $p_{fission}$ values have random errors from the Monte Carlo process and possibly an overall bias from errors in the MCNP model. The random error is calculated by MCNP; the bias must be estimated from the quality of the calculated count relative to measured standards. The propagation of these uncertainties follows from the usual statistical process with Eq. (3).

$$\sigma_D{}^2 = \left(\frac{D}{M_{DN}\varepsilon}\right)^2 \cdot \sigma^2{}_{M_{DN}\,\varepsilon} + \sum_{j=1}^{6}\left\{M_{DN}\varepsilon \cdot \left(e^{-\lambda_j \cdot t_r}\right)\cdot\left(1-e^{-\lambda_j \cdot t_C}\right)\cdot\left[\frac{n-(n+1)\cdot e^{-\lambda_j\cdot\tau}+e^{-(n+1)\cdot\lambda_j\cdot\tau}}{\left(1-e^{-\lambda_j\cdot\tau}\right)^2}\right]\cdot\sigma_{P_j(t_i)}\right\}^2 \tag{7}$$

$$\sigma_{P_j(t_i)}{}^2 = \left(Y\cdot\bar{\upsilon}\cdot\beta_j\right)^2\cdot\sigma_{p\,fission}{}^2. \tag{8}$$

The error given by MCNP for an efficiency or multiplication calculated with MCNP can be well under 1% even with short calculation times. The error from modeling inaccuracies can only be judged from comparison with measured efficiencies; these have been shown to be equally small. So an assigned relative error for $M_{DN}\,\varepsilon$ of 0.5% is probably conservatively large.

MCNP also gives uncertainties in each of the $p_{fission}$ values it calculates. These are largest when the ^{252}Cf is farthest from the fissile material. But at distant positions $p_{fission}$ is smaller and less important than when the ^{252}Cf is close to the fissile material. For simplicity, a constant uncertainty closer to the smaller of the stated uncertainties is used in Eq. (8).

The variation in σ_D over a wide range of uranium mass in oxide form was found to be quite small and not much greater than 2% for one set of materials. This used 0.5% for the uncertainty of $M_{DN}\varepsilon$ and uncertainties in $p_{fission}$ from 1.25% to 2.00%.

A STATIC CHECK

If the calculation algorithm is correct, then it should also apply to irradiations where the ^{252}Cf source is stationary. This is the simplest case so a failure in the static mode would guarantee failure with the more complicated scanning mode.

The CMR shuffler and the 125 g of ^{235}U in the U_3O_8 standard were used to perform this check. The ^{252}Cf source was driven at high speed 60, 62, 64,..., or 90 in. and held there for an irradiation period. Then it was rapidly driven to the storage position and a count taken. From these 16 different positions, a response profile is generated showing delayed neutron count rate versus ^{252}Cf distance. The theory was then used to calculate the count rate for the same conditions. The measured and calculated count rates compared essentially perfectly, as shown in Fig. 1. The uncertainties drawn on the measured rates are from counting statistics only. The case with a scanning source is a combination of these static cases, so it should give equally good results.

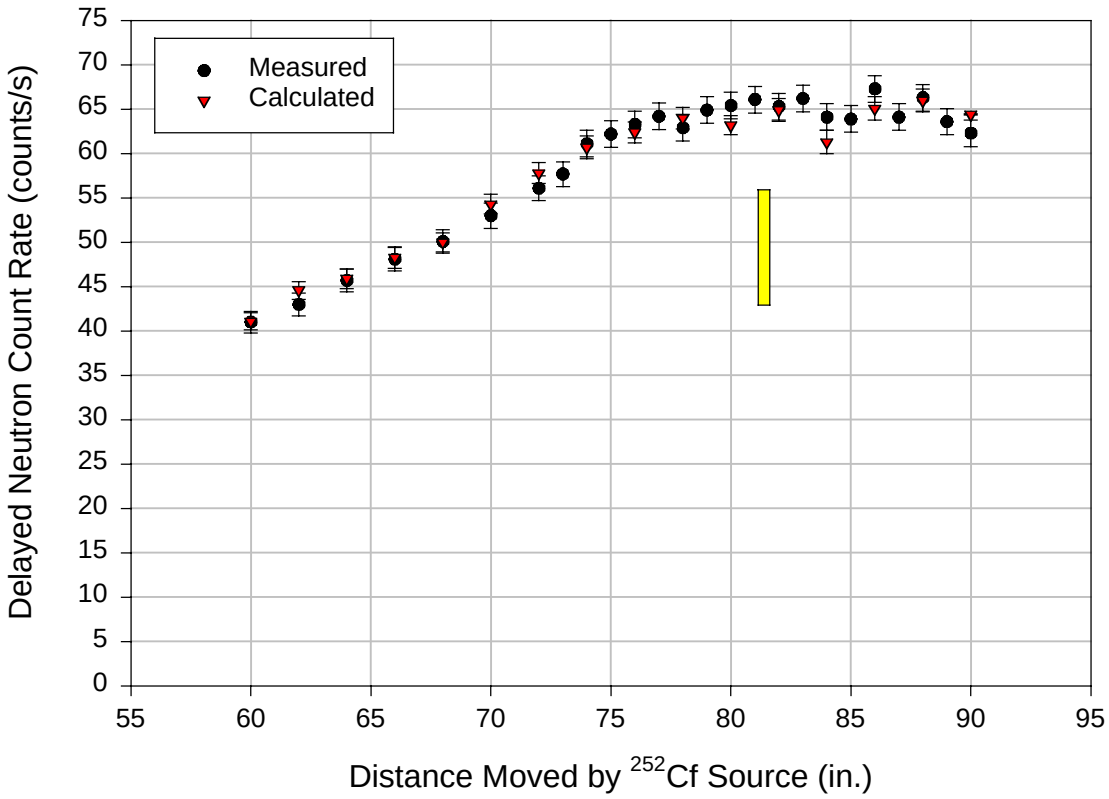

Fig. 1. This shows measured and calculated response profiles for a stationary ^{252}Cf source at different distances from the stored position inside a shield. The vertical rectangle at the 82-in. position shows where the U_3O_8 was and its relative vertical and horizontal dimensions. The 60-in. distance is the top of the assay chamber and the 90-in. distance is near the bottom, so the actual orientation of the U_3O_8 is rotated 90 degrees clockwise from what is shown here.

SPREADSHEET FEATURES

CPS1.XLS

Figure 2 shows most of the spreadsheet CPS1.XLS to be used in problems where the same combination of fissile isotopes is in any number of cells. The fissile isotopes to be used are listed in the upper-left corner under the "1st Cell" label. They must be ordered by atomic number first and then atomic weight. The example in Fig. 2 shows "U-235" followed by "U-238." Another example would be "U-235," "U-238," "Pu-239," and "Pu-240."

Below this list is a box with parameters of the shuffler and the ^{252}Cf source. These must match your shuffler and how it was used during the measurement being simulated by this calculation. The last parameter in that box is the time step used in the numerical integration; 0.001 s is recommended.

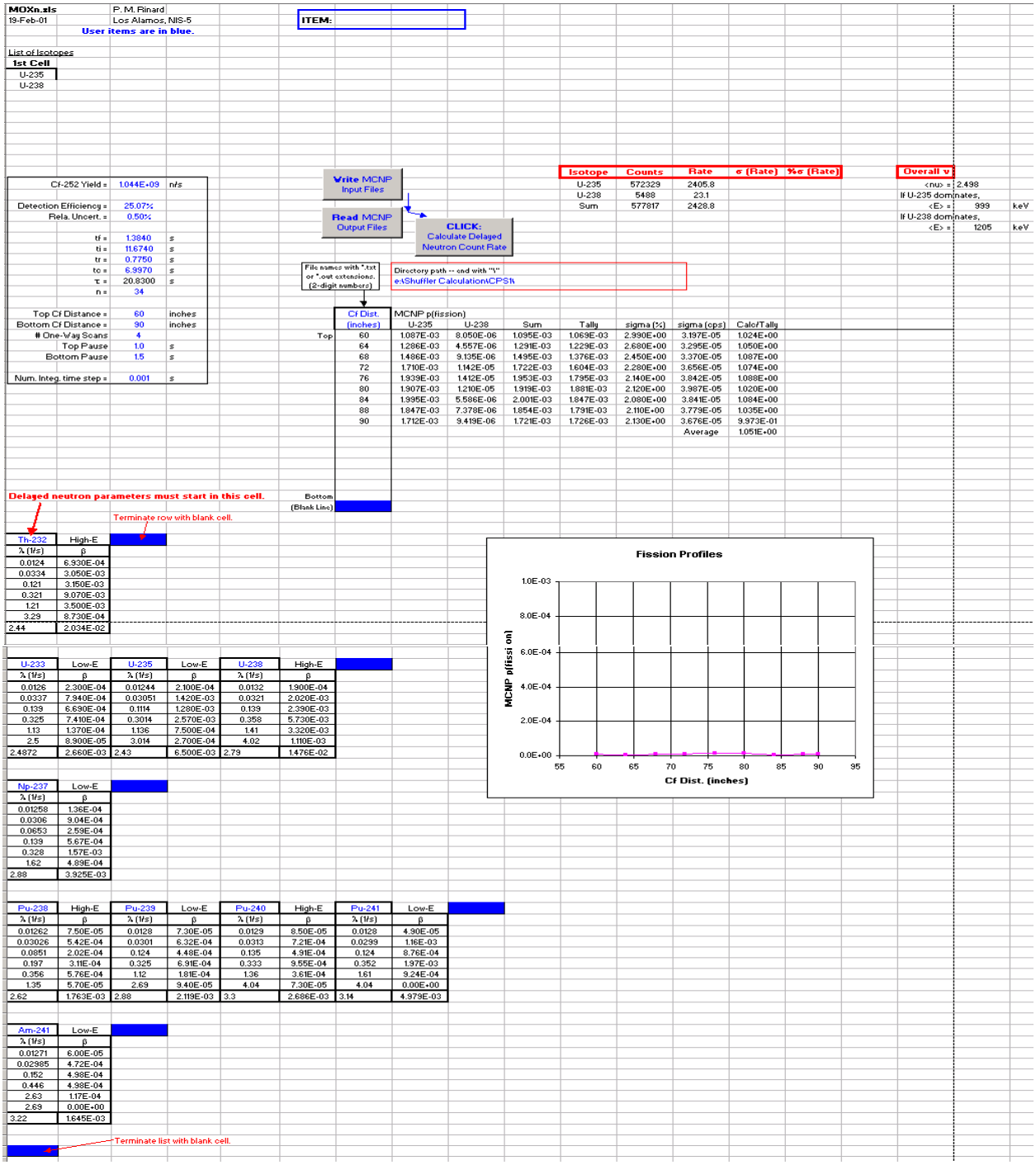

Fig. 2. This is an example of the CPS1.XLS spreadsheet, showing various parameters and results of calculations.

Below this box are delayed neutron parameters for various fissile isotopes. This information must begin in the cell indicated and have two blank rows between sets of parameters. The cells filled with blue are empty and terminate rows and columns. The blue color is unimportant and is used simply to highlight the empty cells. It is not necessary to order the isotopes as shown with a row for each atomic number, but it seems like a logical way to organize the information. If high-energy parameters are to be used rather than low-energy parameters, the user either types in the new values or copies them from similar tables below (not shown in Fig. 2) into this table of parameters. The set of tables of parameters used is terminated with a blank cell two rows below the parameters for the last isotope.

At the top center of the spreadsheet is a cell where a description of the item may be entered. This is not used in any way by the calculations, so using this cell is entirely optional.

The list of ^{252}Cf distances is entered in the cells below the cell containing "Cf Dist. (inches)." This list is terminated with a blank cell. The cell filled with blue is simply a reminder to have a blank cell and has no real significance.

File names have *.txt or *.out extensions after 2-digit numbers that are the Cf distances. The *.txt files are MCNP input files. The user has to create one file with the name of the first Cf distance in the list of distances; in this example it would be "60.txt." The other input files are created automatically and given names with the rest of the Cf distances. For example, "64.txt," "68.txt," down to "90.txt." The distances in the example of Figs. 2 are 4 in. apart between 60 and 88 in. and then a 90 in. distance. There is no requirement that the distance step be constant, so if $p_{fission}$ has a small region of rapid change, additional distances could be given that cluster around that region.

For the two LANL shufflers, I correlated the distance the ^{252}Cf source has moved and the height of the source above the assay chamber's floor. This depends on the length of the Teleflex cable, so the correlation could be a little different even for another shuffler of the same design. The key distance is how far the source moves to reach the floor of the assay chamber; in our case, it is 94.2 in. (2 in. beyond the forward overtravel sensor). This was measured by inserting a short section of Teleflex cable into the guide tube from the opening just above the floor. By marking this cable's position and moving the source a known distance (with the doors closed) to push the short cable a bit, the height of the source above the floor is measured.

Figure 3 tries to clarify the relationship between "distance" and "height" as used here. "Distance" increases downward as the source moves farther from the store position; "height" increases upwards.

So a distance of 94.2 in. corresponds to 0 cm for the MCNP model. A distance of 60 in. corresponds to (94.2 – 60) _ 2.54 = 87.88 cm. The Excel spreadsheets do this calculation to get the variable "CfHeight" but also add 0.8 cm because the ^{252}Cf is that far up from the tip of the source capsule.

The working directory and path must be entered in the cell shown and end with "\". MCNP input files will be written to this location when the "Write MCNP Input Files" button is clicked and MCNP output files will be read from that location when the "Read MCNP Output Files" is clicked.

After the MCNP input file for the first distance has been prepared, click on the "Write MCNP Input Files" button. This will generate the rest of the MCNP input files, using the list of Cf distances you have given. It is not necessary that the correct height be given for the ^{252}Cf source in "60.txt"; CPS1.XLS will rewrite "60.txt" with the right height.

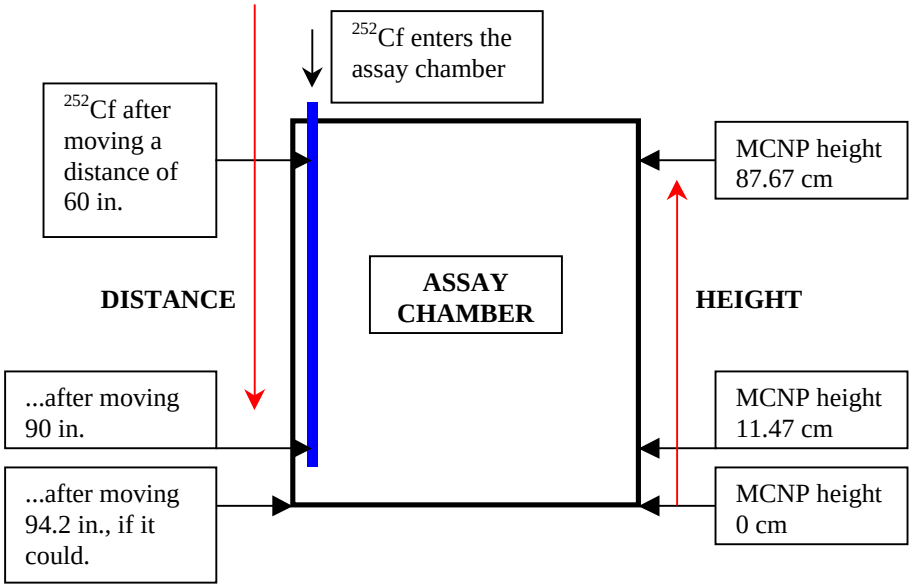

Fig. 3. The assay chamber is viewed from the side; the guide tube for the ^{252}Cf source enters from the top-left. The relationship between "distance" and "height" is given.

At this point, MCNP needs to be run for each of these input files. A batch file was almost generated as the MCNP input files were generated. The "batch.doc" file only needs to be stored as a text file with the extension *.bat. This simplifies doing the MCNP runs on a single computer.

After the MCNP output files have been put in the designated directory, the "Read MCNP Output Files" button is clicked on and the results for all the files are read automatically. Pertinent information is placed in the spreadsheet.

The calculation is performed when "Click: Calculate Delayed Neutron Count Rate" is clicked. The results are shown for each isotope along with their sum. The MCNP output file table labeled "total over all cells for each nuclide" is used to get fission probabilities for all the isotopes. When there is only one isotope, the MCNP fission tally is also used, but this fission rate will include any other fissile isotopes that were not listed in the upper-left corner of the spreadsheet. For example, you may specify only "U-235" but the tally will include fissions in "U-238." Only the delayed neutron parameters for "U-235" will be applied, so the "U-238" must be a minor component of the total if the result is to be accurate. If you specify "U-235" and "U-238," then you get individual fission rates and their sum. The sum should be nearly the same as the tally found when "U-235" was used alone. If the same fissile material is in more than one cell, the tally should include all these cells; the individual fission rates will be for all such cells.

When the cell(s) have a single fissile isotope, the fission tally gives the probability that a single neutron will induce a fission in that isotope. The calculation searches for "multiplier bin:" as it appears in the reproduction below. The line after this key has the tally and its relative uncertainty, shown in bold here.

```
+                                    <<<<< Fission Probability Per Source Neutron >>>>>
           tally type 4    track length estimate of particle flux.
           tally for  neutrons

           volumes
                   cell:     11000
                         1.00000E+00

 cell  11000
 multiplier bin:  -1.00000E+00    5         -6
                 9.29523E-04 0.0141
```

The value and its uncertainty are written into the cells on the same line as the corresponding Cf distance value. The MCNP uncertainty is a percent, so the absolute uncertainty is calculated automatically in the last column of the table. The $p_{fission}$ values are also plotted on the spreadsheet. The curve should be fairly smooth, although for small items there can be more rapid variations when the source is near the item.

If there is more than one fissile isotope in the cell, the tally gives the fission probability for all isotopes combined. No single set of delayed neutron parameters is suitable; an average calculated with weighting factors based on fission probabilities would work if such a scheme could be implemented. At present the tally is simply not used when there is more than one fissile isotope in a cell.

Individual fission rates of the two fissile materials are needed, but MCNP tallies fission rates for whatever is in a cell or cells, which in this case have the two materials combined. Without modifying MCNP, the individual tallies can still be found within a few percent or better. An output file is searched for the key phrase “total over all cells for each nuclide” which heads a list of “weight gain by fission” values for the different isotopes. The list is searched for “92235” and “94239” (if these are the two fissile materials involved) and the two weight-gain values are read for these two isotopes (shown in bold in the following example). The cross-section library designator (e.g., “.50c”) is ignored by the spreadsheet.

total over all cells for each nuclide	total collisions	collisions * weight	weight lost to capture	**weight gain by fission**	weight gain by (n,xn)
1001.50c	453688340	1.0273E+02	5.2707E-01	0.0000E+00	0.0000E+00
2003.50c	678805	1.7983E-01	1.7961E-01	0.0000E+00	0.0000E+00
6000.50c	27112063	6.8200E+00	3.0217E-03	0.0000E+00	0.0000E+00
8016.50c	394877	1.1439E-01	4.5414E-05	0.0000E+00	0.0000E+00
11023.50c	4023	1.2523E-03	4.9017E-05	0.0000E+00	0.0000E+00
12000.50c	5540	1.6633E-03	1.0885E-05	0.0000E+00	0.0000E+00
13027.50c	14223	5.2131E-03	5.5076E-05	0.0000E+00	0.0000E+00
20000.50c	90931	2.5659E-02	1.6584E-03	0.0000E+00	0.0000E+00
26000.55c	13249107	4.5402E+00	7.2822E-02	0.0000E+00	6.2536E-05
48000.50c	1005905	3.2312E-01	1.9536E-01	0.0000E+00	1.9499E-05
92234.50c	78	2.8457E-05	8.0794E-06	4.9338E-06	0.0000E+00
92235.50c	7053	2.5860E-03	2.5551E-04	**1.0766E-03**	1.3857E-06
92236.50c	35	1.3036E-05	4.1870E-06	0.0000E+00	0.0000E+00
92238.50c	383	1.3839E-04	1.8354E-05	4.3010E-06	3.9699E-07
94239.55c	1810	6.5801E-04	7.6290E-05	**3.9378E-04**	0.0000E+00
94240.50c	244	8.4277E-05	5.3611E-05	2.2958E-06	0.0000E+00

The fission probability $p_{fission}$ for each of the isotopes is simple to calculate from (weight gain)/($\bar{\nu} - 1$). The denominator is the net gain in the number of neutrons after an induced fission. The weight gain is the probability that a fission occurs times the number of neutrons gained, as long as neutron importances are set to unity in the MCNP input file. But the average number of fission neutrons is slightly energy dependent and therefore strictly speaking varies from problem

to problem. We cannot use the standard MCNP output to give individual $\bar{\nu}$ values, so the values you set in the spreadsheet are used.

The CPS2.XLS spreadsheet performs a check on the consequences of using the constant $\bar{\nu}$ values you choose. MCNP directly provides the $p_{fission}$ tally for the combination of fissile isotopes. The individual values of $p_{fission}$ calculate from the "weight gain" table are added and compared with the MCNP value. The two may differ by a few percent because of inaccuracies in the specified $\bar{\nu}$ values for the individual isotopes. Some combination of $\bar{\nu}$ values can be found that makes the two total $p_{fission}$ values equal, but so will many other combinations. Without some additional information, there is no informed way to adjust the two $\bar{\nu}$ values.

To the right of the calculated count rates is a cell where a calculated value of $\bar{\nu}$ is shown; this is the weighted average for all fissile isotopes in the MCNP model. The MCNP "ledger" table is read to get neutron gains and losses for a ^{252}Cf position. The number of losses to fissions is the number of fissions. The neutrons gained by fission are all the fission neutrons released by fissions. The ratio of these two ledger values is the average number of fission neutrons per fission. The $\bar{\nu}$ shown is the average of the individual values over all ^{252}Cf positions.

Below is an example of a ledger, divided into two sections to fit on the page. The key items are in bold and show the weight gain and loss from fission. If the MCNP calculation has been "analog," then weight is the same as number of neutrons. Weight or neutrons are lost when neutrons induce fissions after being absorbed. Weight or neutrons are gained when a fission event releases prompt and delayed neutrons.

neutron creation	tracks	weight (per source particle)	energy
source	940892	1.0000E+00	2.3087E+00
weight window	0	0.	0.
cell importance	0	0.	0.
weight cutoff	0	1.1213E-01	8.0516E-06
energy importance	0	0.	0.
dxtran	0	0.	0.
forced collisions	0	0.	0.
exp. transform	0	0.	0.
upscattering	0	0.	5.4180E-07
(n,xn)	184	1.7989E-04	1.5409E-04
fission	6134	**5.0853E-03**	1.0320E-02
total	947210	1.1174E+00	2.3192E+00

neutron loss	tracks	weight (per source particle)	energy
escape	25175	2.1673E-02	1.9265E-02
energy cutoff	0	0.	0.
time cutoff	0	0.	0.
weight window	0	0.	0.
cell importance	0	0.	0.
weight cutoff	919452	1.1186E-01	1.5799E-07
energy importance	0	0.	0.
dxtran	0	0.	0.
forced collisions	0	0.	0.
exp. transform	0	0.	0.
downscattering	0	0.	2.2700E+00
capture	0	9.8171E-01	2.7793E-02
loss to (n,xn)	92	8.9947E-05	1.1955E-03
loss to fission	2491	**2.0579E-03**	1.0144E-03
total	947210	1.1174E+00	2.3192E+00

For a single fission, the average gain is $\bar{\nu}$ and the loss is 1; the average neutrons created per neutron lost (i.e., number of fissions) is $\bar{\nu} = \bar{\nu}/1$. The ledger's weight gains and losses are in the same ratio as $\bar{\nu}$ to 1 for analog problems. So $\bar{\nu}$ = (weight gain)/(weight loss) = 5.0853E-3 / 2.0579E-03 = 2.471 for the problem with the above ledger.

If the number of fission neutrons produced for different energies is known, the average energy of neutrons inducing fissions can be calculated. Reference 3 has conveniently tabulated this information for five important nuclei. Table II displays that information.

Table II. $\bar{\nu}(E)$

Isotope	$\bar{\nu}(E)$	E range (MeV)
^{232}Th	1.873 + 0.164 E	all E
^{233}U	2.48 + 0.075 E	0 ≤ E ≤ 1
	2.41 + 0.136 E	E > 1
	2.45 + 0.126 E	all E
^{235}U	2.432 + 0.066 E	0 ≤ E ≤ 1
	2.349 + 0.150 E	E > 1
^{238}U	2.304 + 0.161 E	all E
^{239}Pu	2.867 + 0.148 E	0 ≤ E ≤ 1
	2.907 + 0.133 E	E > 1
	2.874 + 0.138 E	all E

In the uranium problem shown above, $\bar{\nu}$ = 2.471. This corresponds to an energy of (2.471 – 2.432) / 0.66 = 0.591 MeV, according to Eq. (9). Experience so far has shown that E ranges from 200 to 1000 keV and that the calculated $\bar{\nu}$ is within a few percent of the thermal value.

CPS2.XLS

The spreadsheet CPS2.XLS is shown below as Fig. 4. It is used for different fissile materials (^{235}U and ^{239}Pu in this case) in two different cells. Two tallies are taken, one for each cell. More than one cell may contain the same fissile material as long as the tally includes all the cells with the same material. The steps to use this spreadsheet are similar to that just described for CPS1.XLS but the delayed neutron parameters to be used are placed in the upper-left corner instead of the isotope names. (The version of CPS2.XLS described here is in a less advanced state that CPS1.XLS and eventually may be changed to match the style of CPS1.XLS).

The MCNP input file must have separate fission tallies for each fissile material. The uranium tally must precede the plutonium tally in this example because it is on the left in the spreadsheet sets of parameters and red boxes of results. Below is an example of MCNP input lines that produce two tallies like those shown in Fig. 4, one for each fissile material.

```
fc14   <<<<< Fission Probability Per Source Neutron: U >>>>>
f14:n  10001
fm14   -1 5 -6
sd14   1
c
fc24   <<<<< Fission Probability Per Source Neutron: Pu >>>>>
f24:n  10002
fm24   -1 8 -6
sd24   1
```

The U and Pu are in different cells (10001 and 10002) and have different material numbers (5 and 8). Otherwise, the two tally definitions are the same. The calculated count rates are shown for the two cells along with their sum, all highlighted by red boxes.

It is again possible to use the ledger to calculate a $\bar{\nu}$ but now this is the value for both fissile isotopes in both cells combined. This average $\bar{\nu}$ has no important use in CPS2.XLS. It should be between the two individual $\bar{\nu}$ values and the weighting factors for the two elements' individual $\bar{\nu}$ values can be calculated. But this limited bit of knowledge does not help us determine more accurate $\bar{\nu}$ values for the two isotopes.

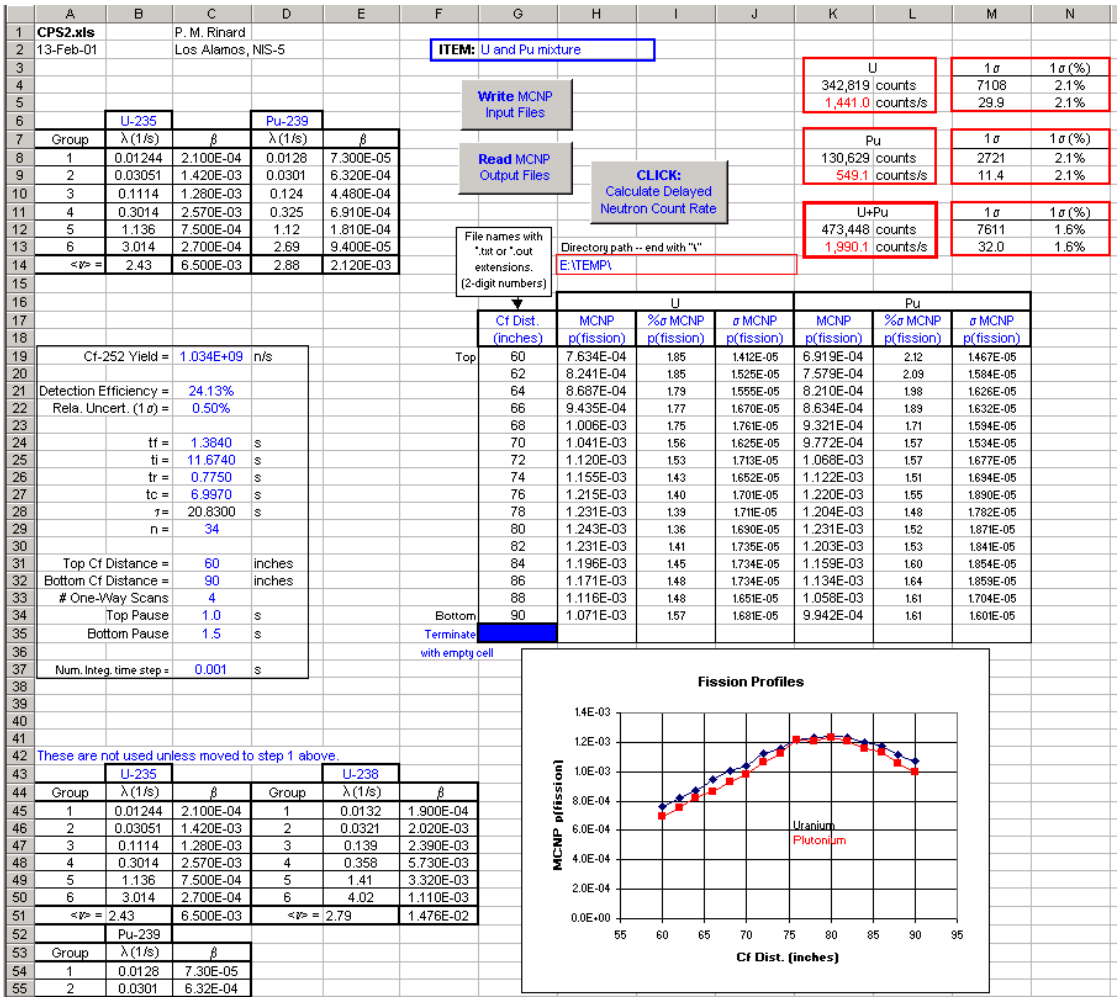

Fig. 4. This is an example of the spreadsheet CPS2.XLS for a combination of uranium and plutonium in different MCNP cells. The value of $\bar{\nu}$ calculated from the ledger is not shown in this example.

^{252}Cf NEUTRON YIELD

The neutron yield *Y* of a shuffler's ^{252}Cf source is usually known only approximately. In practice, the yield need not be known because the calibration takes it into account automatically. One source fabricator assigns an uncertainty of 10% to his stated yield. As shown by Eq. (3), the yield affects a calculated count rate in a direct and simple way: if the yield is in error by 10%, the calculated rate will also be in error by 10%. So the calculational process needs to use an accurate yield even though the empirical calibration with physical standards does not.

If would be best if the yield could be directly measured by an accurate neutron counting technique. If this cannot be done, one or more items need to measured in the shuffler and used to deduce the yield. If the same yield gives accurate count rates for a variety of standards, it must be correct.

At LANL we have measured a large number of U_3O_8 certified standards and the measured count rates can be reproduced accurately by calculation. However, there are two free parameters in this case: oxide density and yield. The density is more poorly known than the yield, and many combinations of density and yield can be found that will produce the same count rate.

We have also measured some well-characterized metal objects where the densities are known with much more certainty. These have been used to find neutron yields that have small uncertainties. (Reference 2 discusses some of the work with metals.)

The same yield must apply to all materials and indeed only a very narrow range of possible yields satisfies all the LANL data (oxide and metal). The yield is still has a within a one or two percent uncertainty because there are measurement and calculational errors of that size. But the fact that one yield applies to all the different measurements indicates that the calculational process is correct.

DETECTION EFFICIENCY

The reported detection efficiency of neutron instruments is usually measured by placing a ^{252}Cf source with a known emission rate in the center of an empty assay chamber. The measured count rate divided by the emission rate is the detection efficiency. This is *not* appropriate for shufflers because delayed neutrons have lower average energies than prompt fission neutrons, and the object being measured can modify the detection efficiency. For example, if the detection efficiency with a ^{252}Cf source is found to be 19%, the detection efficiency with delayed neutrons is about 24%. For an absolute calculation of count rates, this difference is enormous.

There are two ways we have used to get the delayed neutron detection efficiency. MCNP can calculate it after starting neutrons with the energy spectrum of delayed neutrons. The following simple MCNP-ready spectrum (given in the "si1" and "sp1" lines) has been used for shuffler work for many years. It peaks at about 400 keV and the tail stretches to 2 MeV.

```
c    <<<<< Delayed Neutron Source after Fissions Are Induced >>>>>
c
c    sdef   erg=d1 pos=0 0 40.7185 axs=0 0 1  ext=d2 rad=d3  cel=10000
c    si1    h 0 0.30 0.40 0.50 0.60 0.70 0.80 1.20 1.60 2.00
c    sp1    d 0 1.80 1.65 1.35 1.05 0.75 0.45 0.25 0.15 0.05
c    si2    h 0.4185
c    si3    h 0.0 5.0
```

Alternatively, the detection efficiency can be measured for a known AmLi source and used for delayed neutrons because the energy spectra for AmLi neutrons is nearly the same as for delayed neutrons. The difficulty here is to get an AmLi source with an emission rate known to better than 1%.

The detection efficiency can be affected by the matrix material in the item being assayed. The energy spectrum of neutrons leaving oxide differs from that for neutrons from metals. The detection efficiency can be affected by a few percent. A large amount of moderator will strongly affect the fission rate and therefore the production rate of delayed neutrons, but it will also affect the energies of delayed neutrons that escape the item.

DENSITY EFFECTS

The most common uranium standards are oxides, generally U_3O_8. These can be well characterized through chemistry during fabrication. The problem with oxides is that the density of the powder is not a constant. Shaking a container will loosen the grains, reducing the density. Tapping the container on a table, or just letting the container sit quietly on a shelf for days or weeks, will pack the grains together and raise the density.

For example, a can with 2800 g of ^{235}U in U_3O_8 was measured after shaking and tapping; the change in the measured count rate was 3%. This is not a huge change, but if you are trying to do precise, reproducible work, this is rather large.

The best that can be done is to handle cans of powder in a reproducible way that minimizes the changes in density between measurements. This approach has been quite successful at LANL as the same powders are used successfully for daily measurement control checks.

Applying the best estimate for the neutron yield in calculations shows that the best estimate of the oxide density is 4 g/cm^3 when handled in the standard manner. Densities of 3 g/cm^3 and 5 g/cm^3 require a 5% change in the neutron yield, making the yield incompatible with yields needed for metals. So the oxide density is probably bounded by 3.9 and 4.1 g/cm^3.

The density of metals can vary also. One mechanism for a density change is micro-cracking that increases the volume. Calculations show that a density change from 19 g/cm^3 to 16 g/cm^3 affects the count rate by about 1.3%.

MODIFYING AND USING THE MCNP INPUT FILES

A step-by-step check list for performing the calculations is given in the Appendix. This section has details and examples about the key sections of the input files, along with an example of a batch file and hints on run times.

Most of the MCNP input file for the 55-gallon drum shuffler remains unchanged from calculation to calculation because describing the shuffler body occupies most of the input file. But some of the lines describe the fissile bearing item. The stand on which the item rests should be modeled accurately also, especially the portions adjacent to the item. If the item rests on a metal plate, that plate scatters some neutrons away instead of entering the bottom of the item, and the effect is noticeable.

Here are the sections of the MCNP input file that generally require modifications for different items. They are blocked off by double lines to help you find them in the file.

1. Assay Chamber Void Cell

This describes the assay chamber surrounding the item being assayed. It is a void region. This copy from the file has three choices: an empty assay chamber, a 55-gallon drum for the item, and a can on top of the LLNL pedestal. Two of these choices are always deselected by making them comment lines. If they are of no interest at all, they can simply be deleted. If consistent use is made of the outermost surface numbers from item to item, namely (13002 : 13004 : –13003), these lines need not be changed for a different can.

```
c    ===================================================================
c    ===================================================================
c
c    Assay chamber void regions around assorted items inside
c
c
c    Choice #0.  Empty Assay Chamber.
c
c    999    0 (-602  -607  -605  -606  601  -603  -604  100  -200)
c                                    imp:n=1
c
c    Choice #1.  55-gallon drum.
c
c    999    0 (-602  -607  -605  -606  601  -603  -604  100  -200)
c        (10000 : -10001 : 10002)              imp:n=1
c
c
c    Choice #2.  LLNL pedestal with can of fissile material.
c
999    0 (-602  -607  -605  -606  601  -603  -604  100  -200)
       (-12044 : 12045 : -12041 : 12042)     $ ring
       (-12040 : 12041 : 12051)              $ lower rods
       (-12040 : 12041 : 12052)
       (-12040 : 12041 : 12053)
       (-12040 : 12041 : 12054)
       (-12042 : 12043 : 12051)              $ upper rods
       (-12042 : 12043 : 12052)
       (-12042 : 12043 : 12053)
       (-12042 : 12043 : 12054)
       ( 13002 : 13004 : -13003)             $ Fissile material can outer surfaces
                imp:n=1
c
c    ===================================================================
c    ===================================================================
```

2. Cells for the Item Being Assayed

This includes the stand on which the item rests; in this example, it is a LLNL shuffler stand. The only parts that change from can to can are cells 13001 and higher. This example has some carbon felt at the top of the item, which is not commonly present. The list of material specifications may need modification if new materials are involved.

```
c     ===================================================================
c     ===== Put Your Item Here ==========================================
c
c      Item inside the assay chamber:  pedestal and LLU
c
12011  3 -7.87 12044 -12045 12041 -12042   imp:n=1   $ ring
c
12021  3 -7.87 12040 -12041 -12051        imp:n=1   $ lower rods
12022  3 -7.87 12040 -12041 -12052        imp:n=1
12023  3 -7.87 12040 -12041 -12053        imp:n=1
12024  3 -7.87 12040 -12041 -12054        imp:n=1
c
12031  3 -7.87 12042 -12043 -12051        imp:n=1   $ upper rods
12032  3 -7.87 12042 -12043 -12052        imp:n=1
12033  3 -7.87 12042 -12043 -12053        imp:n=1
12034  3 -7.87 12042 -12043 -12054        imp:n=1
c
13001  3 -7.6 13001 -13002 13003 -13004   imp:n=1  $ Bottle side
13002  3 -7.6 -13001 13003 -13011          imp:n=1  $ bottom
13003  8 -0.09807 -13001 13012 -13013     imp:n=1  $ carbon felt
13005  3 -7.6 -13001 13013 -13004          imp:n=1  $ top
c
13010  0      13031 -13012 -13001       imp:n=1  $ void above fissile stuff
13011  5 -2.4 13011 -13031 -13001     imp:n=1  $ CRM-149 U3O8
c
c
c     ===================================================================
c     ===================================================================
```

3. Surfaces for the Item Being Assayed

The cells of the void (999) and of the item inside the assay chamber (cells 13001-13011 in the previous example) are specified by surface numbers. The surfaces with those numbers must be given later in the input file. They are grouped between dashed lines at the bottom of the list of surfaces, just above the material specifications. Here are the surfaces that match those used by the cells in paragraph 2.

```
c     ====== Put the Item Here ========================
c
12041   pz 48.34         $ring of the LLNL stand
12042   pz 48.96
12044   cz 18.30
12045   cz 23.60
c
12040   pz 0.01          $ lower rods of the LLNL stand
12043   pz 60.96         $ upper rods of the LLNL stand
12051   c/z  15.27  15.27 0.635
12052   c/z -15.27  15.27 0.635
12053   c/z -15.27 -15.27 0.635
12054   c/z  15.27 -15.27 0.635
c
13001   cz 2.17         $ side of container
13002   cz 2.465
13003   pz 48.9601
13004   pz 71.8201
13011   pz 49.4901    $ bottom of fissile
13012   pz 70.1101    $ top of fissile
13013   pz 70.7401
c
c     ================================================
```

Surfaces with numbers in the 12000s are for the stand and rarely change for a given shuffler. Surfaces in the 13000s are for the container and fissile material. Here it is a vertical cylindrical container so there are only cylindrical surfaces about the *z* axis sliced by planes perpendicular to the *z* direction to define the top and bottom.

4. Source Definition

The source definition line, "sdef," gives the position of the ^{252}Cf source, among other things. This line *must* end with "z=nnn", where "nnn" is some number. See the example below.

```
c     Stationary Cf-252 Source
c
sdef   erg=d1 x=0 y=38.8113 z=87.67
sp1    -3 1.025 2.926
```

It does not matter what "nnn" is in the first input file (e.g., "60.txt") because it will be changed to match the entry in the list of file names given in the spreadsheet. But the "sdef" is parsed for the "=" sign starting from the right end and working to the left. If "z=nnn" is not at the end of the line, the wrong variable will be changed.

5. Fission Probability Tally

If the cell with the fissile material is always given the same number and the fissile material always has the same material number, this tally doesn't need to be changed. The cell number is "13011" in the "f4:n" line of the example below. If another cell has the fissile material, put its number in place of "13011." The material number is "5" in the "fm4" line. Put your own material number here if it is not "5."

```
fc4   <<<<< Fission Probability per Source Neutron >>>>>
f4:n  13011
fm4   -1 5 -6
sd4   1
```

Note that if the wrong material number is used (something other than 5 in this case), fissions in that material with the density given for cell 13011 will be tallied. If that other material is aluminum, for example, there won't be any fissions. If you have the material correct but the wrong cell number (e.g., 13001), there will be a fission tally as if that cell had the fissile material with the density given for that cell. This last case is difficult to detect because the tally is nonzero.

The "fm" line also specifies that the density given for that cell will be used (-1) and that fissions will be counted (-6).

The "sd" line is very important. If it were not present, the tally would be divided by the volume of the cell. The parameter "1" means that the tally will be divided by unity instead.

The "fc" card is merely a comment that you can customize. It is repeated on the printout just before the tally is given. A comment card is not required.

6. Detection Efficiency

If you need to calculate the detection efficiency for the delayed neutrons started within the item, comment out or delete the fission tally (shown in paragraph 5 just above) and remove the comment symbols and spaces before the following lines of another tally for the (n,p) production in ^{3}He tubes. The "nonu" line prevents any of the delayed neutrons from inducing a fission during this calculation. We do not want any prompt fission neutrons confusing the issue of the detection efficiency of delayed neutrons.

```
c
c     fc4   <<<<< Detection Efficiency >>>>>
c     f4:n  (201 202 203 204 205 206 207 208 209 210 211 212
c           301 302 303 304 305 306 307 308 309 310 311 312
c           1001 1002 1003 1004 1005 1006 1007
c           1011 1012 1013 1014 1015 1016
c           1021 1022 1023 1024 1025 1026
c           1031 1032 1033 1034 1035 1036 1037
c           1041 1042 1043 1044 1045 1046 1047
c           1051 1052 1053 1054 1055 1056 1057)
c     fm4   -1 4 103
c     sd4   1
c     nonu
c
```

The parameters in the "f4:n" line appear as the list of ^{3}He detector cells. They are combined into one tally by placing them inside parentheses.

The "fm" card says to use the density of the cell (-1), the material number (4) that corresponds to ^{3}He, and tally (n,p) reactions (identified for MCNP as 103).

For a detection efficiency calculation, the source definition must be changed to start delayed neutrons within the item. For cans of oxide, neutrons are started throughout a cylinder coincident with the powder. Below is an example. The fissile material is in cell 11000 with the dimensions specified by the "pos," "axs," "ext," and "rad" parameters.

```
c     <<<<< Delayed Neutron Source after Fissions Are Induced >>>>>
c
sdef   erg=d1 pos=0 0 30.31549 axs=0 0 1  ext=d2 rad=d3  cel=11000
si1    h 0 0.30 0.40 0.50 0.60 0.70 0.80 1.20 1.60 2.00
sp1    d 0 1.80 1.65 1.35 1.05 0.75 0.45 0.25 0.15 0.05
si2    h  0.29149
si3    h  0.0  6.3534
c
```

The "si1" and "sp1" lines referred to by "erg" specify the energy spectrum of delayed neutrons as a histogram. The "pos" dimensions give the center of the cylinder. The "axs" gives direction cosines of the cylinder's axis. The "si2" parameter gives half the height of the cylindrical source in the axial direction. The "rad" parameters are the minimum and maximum radii of the source.

This is simplest geometry to use in starting delayed neutrons, but it is an approximation. Probably more fissions occur near the cell's surface than near its center, and more delayed neutrons should be started near the surface also. The best way to do this is to modify MCNP to generate a file with coordinates of locations where fissions occur. Then the detection efficiency calculation reads this file and starts delayed neutrons at the same positions. This approach has been used in the past, but the standard MCNP code does not provide a way to do it. An approximate way is to use a formula for starting positions that are weighted toward the surface. The MCNP manual describes ways to modify the starting locations from the uniform distribution shown in the above example.

7. Multiplication

There are actually two separate neutron multiplications in these calculations. The first occurs during an irradiation when prompt fission neutrons induce additional fissions that create additional delayed neutron precursors. This multiplication is automatically included in the calculation of $p_{fission}$. The second occurs when delayed neutrons induce fissions during the counting time; this is M_{DN} and is the subject of this section.

The process of calculating M_{DN} starts neutrons throughout the fissile material with the energy spectrum of delayed neutrons. Tallies are then calculated from the number of first-generation neutrons released during fissions induced by the delayed neutrons and from the number of second-generation neutrons created by first-generation neutrons' fissions.

$$M_{DN} = \frac{\nu_1 \cdot f_1 - f_2 + \nu_2 \cdot f_2}{\nu_1 \cdot f_1} \tag{9}$$

The numerator is the average number of first-generation neutrons created by a single delayed neutron, minus the probability that a first-generation neutron will be absorbed, plus the number of second-generation neutrons created when a first-generation neutron is absorbed. The denominator is again the number of first-generation neutrons created by a single delayed neutron. In short, M_{DN} is the ratio of the number of surviving neutrons from the first and second generations to the number in the first generation, which is the definition of multiplication. These multiplication neutrons are mostly prompt neutrons, but they are emitted during the count time and are indistinguishable from delayed neutrons.

It is convenient to introduce the total fission probability f_T which is $f_1 + f_2$ and also $\nu_T \cdot f_T$ which is $\nu_1 \cdot f_1 + \nu_2 \cdot f_2$.

$$M_{DN} = \frac{\nu_T \cdot f_T - f_T + f_1}{\nu_1 \cdot f_1} \tag{10}$$

MCNP tallies can give us the terms in Eq. (10). One MCNP calculation with two tallies will give f_T and $\nu_T \cdot f_T$; use FMn -1 (m) -6 and FMn -1 (m) -6 -7, where (m) is the material number. A second MCNP calculation with the same tallies plus a "nonu" line will give f_1 and $\nu_1 \cdot f_1$.

These additional calculations are more important as the multiplication grows. But they are important even with small multiplications (≈1.02) when there are variations among the items of interest. For example, U_3O_8 oxides can have ranges from a few grams to several kilograms. The multiplication may never be very large, but including the small changes in multiplications among the items improves the overall results noticeably. For metallic disks of HEU the multiplications are absolutely necessary because they can easily be as large as 1.40. Fortunately, the two MCNP calculations needed can be quite short, often only 5 min long with the present computer speeds.

8. Batch Files

A batch file allows you to run a set of MCNP problems without having to start each one individually when the previous one is finished. I assume that MCNP is being run out of DOS; in that case, the batch file must have the “*.bat” extension. Below is an example that does nothing but start 16 MCNP runs. The easiest way to execute the batch file is simply to double click on it. A DOS window is created automatically and closes when the 16 runs are finished.

```
mcnp inp=60.txt outp=60.out
mcnp inp=62.txt outp=62.out
mcnp inp=64.txt outp=64.out
mcnp inp=66.txt outp=66.out
mcnp inp=68.txt outp=68.out
mcnp inp=70.txt outp=70.out
mcnp inp=72.txt outp=72.out
mcnp inp=74.txt outp=74.out
mcnp inp=76.txt outp=76.out
mcnp inp=78.txt outp=78.out
mcnp inp=80.txt outp=80.out
mcnp inp=82.txt outp=82.out
mcnp inp=84.txt outp=84.out
mcnp inp=86.txt outp=86.out
mcnp inp=88.txt outp=88.out
mcnp inp=90.txt outp=90.out
```

Both of the spreadsheets (CPS1 and CPS2) generate files called "Batch.doc" that are text files. This file can be easily edited if necessary. Changing the extension from *.doc to *.bat makes it a batch file, as long as the file is ASCII. To edit a *.bat file, do not double click on it and expect an editor to appear; the *.bat file will begin execution.

You can use the 16-line batch file to run the 9-file case even though half the input files are not present. If "62.txt" is missing, for example, that MCNP run is not even started and the next command line is executed.

Other lines could be added to automatically erase RUNTPE files, copy "*.out" files into another directory, etc. But the lines shown are the minimum needed to automatically run all 16 problems.

The batch file and input files have to be in the same directory as "mcnp.exe" unless you have set up a special pathway between the executable and the input files. If your computer has two processors, they can be used simultaneously to complete the calculations in half the time. Start two batch files, each having half the input files.

9. Calculation Time and Precision

The longer the MCNP calculation time used, the better is the precision. Some rational compromise between time and precision must be chosen. Getting to 1% precision is always comforting, but if this may require an hour on a high-speed computer. A set of 16 ^{252}Cf positions can therefore be finished in 16 hours. But if 5% precision is satisfactory (as it usually seems to be), the time per calculation might be only 15 min, and 16 such calculations are done in 4 hours.

If a good but quick result is needed, the ^{252}Cf distances can be 4 in. apart (60, 64, 68,...,88, and 90 in.) and 10 min used on each of the nine cases. (The 90-in. distance is needed to define the extreme of $p_{fission}$, so a 2-in. step is used from the 88-in. distance.) The results are ready in only 90 min.

Obviously all this depends on the speed of the computer being used. The examples given are for computers in the 500 to 900 MHz range.

As the step distance is increased, you can expect to get a slightly lower count rate. This is understood from Fig. 6 where the "true" $p_{fission}$ curve, with an infinitesimal step size, is compared to an approximate curve with a finite step size. Linear interpolation is used in the spreadsheet codes so the $p_{fission}$ values will always be slightly smaller than the true values. Experience has shown that going from 2 in. to 4 in. step sizes introduces an error of about 0.5%. In most cases, this is of little importance and is smaller than the error in the calculated count rate from other causes (see the next section).

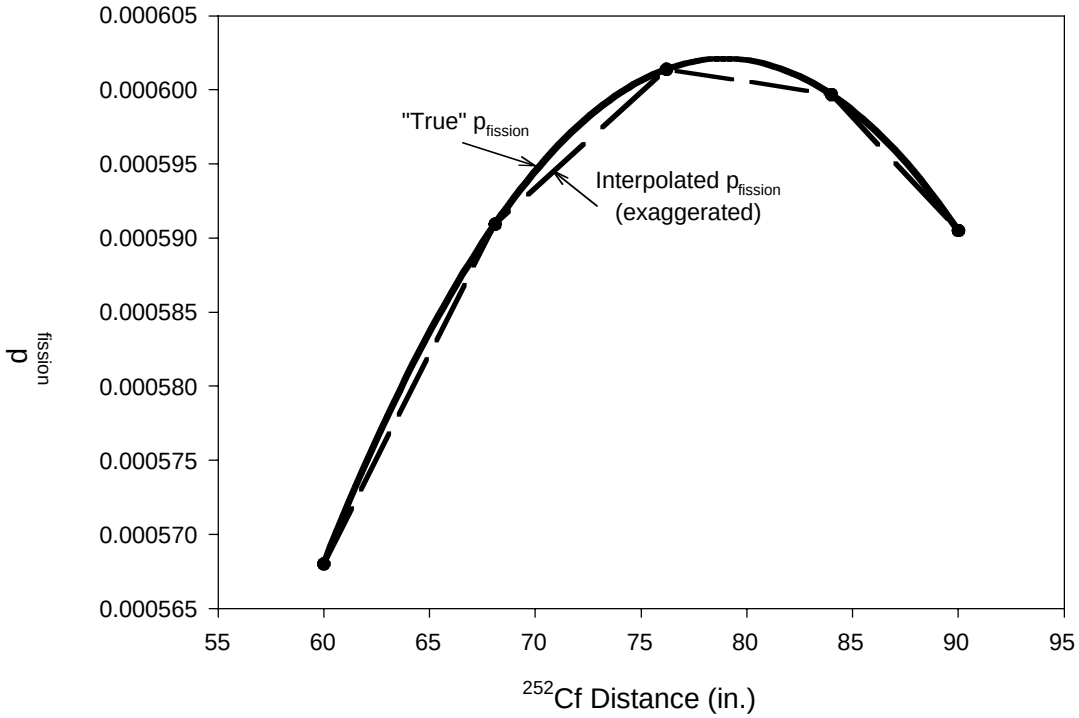

Fig. 6. Linearly interpolated $p_{fission}$ values will be smaller than the "true" values for this type of variation of $p_{fission}$ with ^{252}Cf distance. Note that the step distance had to be made very large (8 in.) to make the effect clearly visible. Even a step of 4 in. gave linear interpolations that are nearly the same as the curve.

An obvious improvement is to use nonlinear interpolation that better fits the shape of the $p_{fission}$ profile. Lagrangian interpolation is commonly used for general shapes, but it fails in this case near the ends, where it oscillates rather wildly. When a better interpolation scheme is found, it will replace linear interpolation.

I have not explored a wide range of times and combinations of distances. I have generally used 16 distances, 2 in. apart, and times long enough to give precisions between 1% and 5%. When I have used 9 distances, 4 in. apart (except for the last pair at 88 and 90 in.), the results have been very satisfactory.

For the very best results, get the fastest computer you can and use the longest times you can afford. An hour on a modern computer is bound to give about 1% precision for all but the smallest masses of fissile materials. And 16 hours of computation time is still only overnight.

UNCERTAINTIES OF CALCULATED COUNT RATES

The uncertainty of a calculated shuffler count rate can be estimated, as is done below. The results give assurance that the uncertainty in a calculation is small, as it should be, given the persistent agreement between calculations and measurements. Each calculation has its own circumstances that contribute to an uncertainty. Two examples (a low and high mass of U_3O_8) will be used here to get insight into the size of the uncertainties that might routinely be encountered. Despite a factor of 22 in the masses, the resulting relative uncertainties are within 50% of each other. This implies that a single uncertainty can be used over a wide range of

materials unless there is some reason to perform detailed uncertainty calculations for every case. The EXCEL spreadsheets perform the calculations described below, so each result has its own uncertainty.

Analysis and Examples	125-g ^{235}U in U_3O_8	2800-g ^{235}U in U_3O_8
Step 1. The MCNP code calculates the probability of a single neutron inducing a fission $p_{fission}$ and a relative uncertainty for it. With a modern computer and an hour or less of calculations, the relative uncertainty is about 2%. The values of $p_{fission}$ depends on the ^{252}Cf positions, but the range is only about a factor of 2 for a given fissile mass. It is important to know the impact of the choice of the ^{252}Cf positions to use in the MCNP calculations. Usually 16 positions spaced 2 in. apart have been used. The resulting count rate is only slightly affected by using 9 of these 16 positions; the gap between positions is now 4 in. except at either the beginning or the end where 2 in. is still used. A less regularly spaced selection from the 16 positions has also been chosen. All the calculated count rates were the same (well within 0.5%). So the choice of ^{252}Cf positions does not have a major effect on the calculated count rate, and it will not be considered further.	$p_{fission}$ = $1.1 \_ 10^{-4}$ to $1.7 \_ 10^{-4}$ $\sigma(p_{fission}) = 2.2\%$	$p_{fission}$ = $2.9 \_ 10^{-3}$ to $1.6 \_ 10^{-3}$ $\sigma(p_{fission}) = 1.5\%$
Step 2. The neutron production rate $f(t)$ at a time t is calculated from the fission probability. $f(t) = p_{fission}(t) \cdot Y \cdot \bar{\upsilon}$ The neutron yield from the ^{252}Cf source Y is taken here to be $1 \_ 10^9$ n/s, corresponding to 427 μg of ^{252}Cf. The average number of fission neutrons $\bar{\upsilon}$ produced is taken as 2.43 (^{235}U). $f(t)$ has a range of values for the different ^{252}Cf positions. The uncertainty of $Y \cdot \bar{\upsilon}$ is taken to be 2%. The uncertainty of $f(t)$ is then calculated by standard error propagation.	$f(t)$ = $2.43 \_ 10^9 \, p_{fission}(t)$ $f(t)$ = $2.8 \_ 10^5$ to $4.2 \_ 10^5$ $\sigma_{f(t)}$ = 3.0% $f(t)$ = $8.4 \_ 10^3$ to $1.3 \_ 10^4$	$f(t)$ = $2.43 \_ 10^9 \, p_{fission}(t)$ $f(t)$ = $4.0 \_ 10^6$ to $7.3 \_ 10^6$ $\sigma_{f(t)}$ = 2.5% $f(t)$ = $1.0 \_ 10^5$ to $1.8 \_ 10^5$

Step 3. The solutions of six differential equations for the delayed neutron group precursor populations are found numerically: $\frac{dP_j}{dt} = f(t)\cdot\beta_j - \lambda_j \cdot P_j(t)$, j = 1, 2, ..., 6 . The uncertainties of β_j and λ_j are taken to be negligible compared to that of *f(t)*. The differential equations are solved by iterations using this expression: $P_j(t+\Delta t) \approx P_j(t) + \Delta P_j(t)$ $= P_j(t) + \left[f(t)\cdot\beta_j - \lambda_j \cdot P_j(t) \right]\cdot \Delta t,$ $P_j(0) = 0$. The iterations are continued until the end of the irradiation at time t_i. The biggest individual uncertainty here is of *f(t)*. Considering the source of this error, it is not random but systematic. As a relative error it will applied to the P_j also because the $\lambda_j P_j(t)$ term is much smaller than the $f(t)\ \beta_j$ term, as must be the case if the precursors to delayed neutrons are to grow rapidly during the irradiations. $\frac{\sigma_{Pj}}{P_j} = \frac{\sigma_{f(t)}}{f(t)}$	$P_1(t_i)$ = 906 ± 27 $P_2(t_i)$ = 5595 ± 170 $P_3(t_i)$ = 3488 ± 100 $P_4(t_i)$ = 3618 ± 110 $P_5(t_i)$ = 282 ± 8.5 $P_6(t_i)$ = 34 ± 1.0	$P_1(t_i)$ = 11020 ± 280 $P_2(t_i)$ = 68070 ± 1700 $P_3(t_i)$ = 42510 ± 1100 $P_4(t_i)$ = 44280 ± 1100 $P_5(t_i)$ = 3490 ± 87 $P_6(t_i)$ = 415 ± 10
Step 4. The delayed neutron precursor populations after the first irradiation $P_j(t_i)$ are used to calculate the count of delayed neutrons D after n irradiations. $D = M_{DN}\varepsilon\cdot\sum_{j=1}^{6} P_j(t_i)\cdot\left(e^{-\lambda_j\cdot t_r}\right)\cdot\left(1-e^{-\lambda_j\cdot t_C}\right)$ $\cdot\left[\frac{n-(n+1)\cdot e^{-\lambda_j\cdot\tau}+e^{-(n+1)\cdot\lambda_j\cdot\tau}}{\left(1-e^{-\lambda_j\cdot\tau}\right)^2}\right]$		

The nuclear parameters and the times are taken to have no significant uncertainties, but the detection efficiency ε is assumed to be 0.5% (1σ) uncertain. $\sigma_D = \left(\frac{D}{\varepsilon}\right)^2 \sigma_\varepsilon{}^2 +$ $\varepsilon^2 \cdot \sum_{j=1}^{6} \sigma_{P_j}{}^2 \cdot \left[\frac{\left(e^{-\lambda_j \cdot t_r}\right)\left(1-e^{-\lambda_j \cdot t_c}\right) \cdot \left(n-(n+1)\cdot e^{-\lambda_j \cdot \tau} + e^{-(n+1)\cdot \lambda_j \cdot \tau}\right)}{\left(1-e^{-\lambda_j \cdot \tau}\right)^2} \right]^2$	D = 57,200 ± 1300 ± 3.0%	D = 701,750 ± 15000 ± 2.5%
<u>Step 5.</u> The relative uncertainty of a count rate $D/(n\ t_c)$ is the same as for the count D. Uncertainties of measured count rates are about 0.5% for high masses and about 1% for low masses, based on standard deviations of repeated measurements. The uncertainty of a single measurement is of course larger (1.0 to 1.5%) The calculated uncertainties are about 2% and larger than the measured uncertainties.	Measured count rate reproducibility = 0.9% $D/(n\ t_c)$ = 240.5 ± 3.0% = 240.5 ± 7.2 counts/s	Measured count rate reproducibility = 0.6% $D/(n\ t_c)$ = 2949.8 ± 2.5% = 2950 ± 74 counts/s

The uncertainties of the count rates are reasonably similar to those of measured rates. This agrees with the fact that carefully performed calculations reproduce measured rates with great accuracy.

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2. P. M. Rinard, “Accountability Quality Shuffler Measurements on Pits,” Los Alamos National Laboratory report LA-13757 (October 2000).

3. G. Robert Keepin, *Physics of Nuclear Kinetics* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1965).

APPENDIX

STEPS IN PREPARING, CHECKING, AND RUNNING A NEW PROBLEM

1. Make a new folder and place in it a template for the MCNP input file (e.g., 60.txt) and a template for the Excel spreadsheet (e.g., CPS1.XLS).

2. Edit the MCNP input file.

a. Accurately define the object's new geometry with new MCNP cells and surfaces.

b. Use the "inverse" of the exterior of that new geometry in the MCNP description of the void cell inside the assay chamber.

c. Define any new material that is being used. A negative amount of an isotope means a weight fraction; a positive amount means an atom fraction.

d. Is this a fission probability calculation or a calculation for detection efficiency? Choose the source definition "sdef" that applies; any other such line should be commented or deleted.

For a fission probability calculation, the "sdef" line gives information about the ^{252}Cf source.

```
sdef   erg=d1 x=0 y=38.8113 z= 67.348
sp1    -3 1.025 2.926
```

The "erg" parameter calls the "sp1" line which specifies a Watt spectrum for ^{252}Cf. The source is located at *x*, *y*, and *z*. The *x* and *y* values should not be changed because they are fixed by the geometry of the shuffler. The *z* value changes among the different calculations. It does not matter what you put in for *z* because a code like "CPS" will put in the value that matches what you specifies in the spreadsheet. Even the *z* value for the first input code, 60.txt, does not have to be correct.

For a detection efficiency case, start neutrons in a region that closely matches the fissile material's region. Here is how to specify a cylindrical region:

```
sdef   erg=d1 pos=0 0 40.7185 axs=0 0 1  ext=d2 rad=d3  cel=13011
si1    h 0 0.30 0.40 0.50 0.60 0.70 0.80 1.20 1.60 2.00
sp1    d 0 1.80 1.65 1.35 1.05 0.75 0.45 0.25 0.15 0.05
si2    h 0.4185
si3    h 0 5
```

The neutron energies are chosen with "erg=d1" that uses "si1" and "sp1". There should be no reason to change these values.

"pos=x y z" is the center of the cylinder given by *x*, *y*, and *z*.

"axs=0 0 1" puts the axis of the cylinder in the *z* direction.

"ext=d2" gives half the height of the cylinder in "si2".

"rad=d3" gives the radius of the cylinder in "si3". There are two radii in the example of "si3": 0 and 5 cm. This means that the radii where neutrons start will be selected from 0 to 5. If the first number is 2 cm, then the radii used will be between 2 and 5 cm (annulus).

"cel=n" specifies the cell where neutrons really start. This physical cell should be entirely inside the cylinder where neutrons may be started.

e. Edit the "ctme" line to specify the time you want to spend on each MCNP run. It would be best to comment out any "nps" line so the calculation will not be terminated early by

reaching the preset number of neutrons started. Alternatively, you could terminate on "nps" rather than time, or you could specify both "ctme" and "nps" so that the termination will take place on whichever is reached first.

3. Check the input file.

a. In a fission probability calculation, the number of the cell containing the fissile material should also be given in the tally for fission probability.

b. Look at the geometry as drawn by MCNP.

(1) Open a DOS window.

(2) Run your input file by "mcnp inp=60.txt ip".

(3) If there are "fatal" errors that prevent a plot being drawn, exit the DOS window and edit the input file to correct the errors.

(4) Run again with "mcnp inp=60.txt ip".

(5) At the prompt, specify the plot parameters on a single command line.

"or x y z" is the origin of the plot at *x*,*y*,*z*.

"ex d" is the distance "d" from the origin to an edge of the plot. Making this a smaller number zooms into the plot and shows more details of the geometry; the labels of cells and surfaces also becomes more clear.

"px s" is a plane perpendicular to the *x* axis and a distance "s" from the origin. Similarly for "py s" and "pz s".

"la s c" turns on or off labels of cells "c" and surfaces "s". A "0" means off; a "1" means on. I start with both off because they tend to obscure the plot. I turn on whatever might help me understand any errors later.

(6) If there are red dashed lines on a cell boundary (or beyond), there is a problem with a surface and neighboring cells. There will also be a multi-line comment in the upper-left corner saying there is an error, but it won't give any helpful information.

(7) Use different cuts through the object (px, py, pz) at different locations to try to find sources of errors. In the shuffler model, there are planes defined at px=0, pz=0; if you draw a plot with "px 0" you will get a red dashed line, but this only means that it had trouble deciding how to split the px=0 plane and this is not a geometry error. Use "px 0.001" instead of "px 0" and that red dashed line should go away.

4. Do a test run.

a. Start a run with "mcnp inp=60.txt outp=60.out". After MCNP has run for a few seconds, mouse click on the "X" box in the upper-right corner of the DOS window. This will kill that window, stopping the MCNP run.

b. Open "60.out" with an ASCII editor (WordPad works well). There is a table ("print table 50") showing cells, volumes, and masses shortly below the input lines. Check the cell with the fissile material and see if it has the mass you expect. Remember that this is the total mass in that cell, including oxygen and other nonfissile elements that might have been specified in the materials line.

c. If there is a message on the DOS window about "lost particles," there is a geometry error. The "60.out" file will give specific information about the one or more lost particles. Look near the bottom of the file or search for the word "lost." The message will give a surface where the problem occurred and the nearby cells. Edit your input file to correct the problem. Replot the geometry, especially in the vicinity of this problem, and see if any red dashed lines appear.

Then redo this test run.

d. For an efficiency calculation, the suitability of the volume where neutrons can be started can be checked. It should be the same as the physical cell, or slightly larger. Do a short run (1000 neutrons, or 0.5 min) and find the neutron ledger in the output file (between "print table 110" and "print table 126"). Near the bottom of this ledger is the "source efficiency" and it should be exactly or very nearly 1.00, implying that neutrons are starting within the cell and not outside of it. (Neutrons started outside the cell are immediately killed and waste time but do not contribute to the result.) If not, redefine the volume where neutrons may start to better match the physical cell with fissile material.

5. Prepare all the MCNP input files for this problem.

a. Open the Excel spreadsheet.

b. Are the delayed neutron parameters in the upper-left corner correct for your fissile material(s)?

c. Are the shuffler parameters correct for your application? The first one is the neutron yield (neutrons/s) from the ^{252}Cf source. Use your best known value here.

d. At the bottom of the parameters is a time step used in the numerical integration. I have found that 0.001 s works very well and I would not change that unless you have a good reason.

e. Edit the "Item" description at the top-center (this is not used by the spreadsheet, so it has no impact on the calculations).

f. Edit the "path" to the files you are using.

g. Edit the list of ^{252}Cf distances in the table below the path. The first distance (e.g., 60) and the last distance (e.g., 90) must match the scan distances used in the shuffler measurements. The distances between these extremes can be anything, in principle. I have generally used 2" steps, but 4" steps seem to give equally good results. If you use 4" steps, you get 60, 64, 68,...,88, 90. The "92" is too big, so make sure it is "90". This illustrates the fact that the steps need not be equal in size. For example, you could use "60, 65, 70, 74, 78, 80, 82, 84, 86, 90". This puts more emphasis on the region near 80" where the fissile material is sitting (I assume). But I have almost exclusively used distances equally spaced by 2" so I know this works well.

h. Click on the VisualBASIC "button" to "Write the MCNP input files." In a second or two there will be a "beep" indicating that they have been written and are in the folder specified on the spreadsheet (step 5.f.).

i. Close the spreadsheet.

6. Run the MCNP input files.

a. A batch file was prepared for the input files you just created. It was given the name "batch.doc" and is not a batch file until you rename it as "batch.bat." The "doc" file is easy to edit simply by double-clicking on it. If you double-click on the "bat" file it will execute by opening a DOS window and perform the commands in the batch file.

b. Copy (not "move") the input files and the batch file to the folder with the MCNP.exe file. If you already have a batch file in that folder and it was created for the same set of input file names, you do not need to copy the new batch file.

c. Double click on the "batch.bat" file and all the MCNP runs will be performed automatically. If the "batch.bat" file has a command line (e.g., "mcnp inp=68.txt outp=68.out") for an input file that does not exist, it will skip that line and continue with the whole list of

commands. For example, I have run input files with 4" distance steps using a batch file created for 2" distance steps. Half the command lines are skipped because the input files do not exist. There is no penalty for being lazy here.

7. Calculate the delayed neutron count rate.

a. After all the MCNP calculations have been done, copy the "*.out" files back to the original folder.

b. Open the Excel spreadsheet and click on the VisualBASIC button to "Read the MCNP output files". The tallies and their relative errors are read into the table; each distance takes a second or less.

c. A plot of these tallies is also made just to the right of the table. Check that it seems plausible. The fission probability should be highest in the vicinity of the fissile material. There may be small statistical "wiggles" in the plot, but it should be generally rather smooth. A dip almost occurs with the source directly opposite the material; I think this happens because the cross section of the material is smallest at this position.

d. Click on the VisualBASIC button "Calculate delayed neutron count rate" and the results appear just to the right of the button.

8. Check the calculation's accuracy.

If the comparison of measured and calculated delayed neutron count rates is not satisfactory, first look in the spreadsheet for a divergence from the measurement conditions.

a. Is the neutron yield of the ^{252}Cf source accurate?

b. Are the shuffler parameters correct?

c. Were the right delayed neutron parameters used?

Is the MCNP model correct?

a. Is the mass of the fissile material correct?

b. Is the material specification correct? Check that the relative amounts are given correctly (negative for weights, positive for atoms).

c. Does the geometry look correct when plotted? If there is even one red line, correct the geometry before doing any calculations.

d. Was anything omitted as a simplification? Hydrogenous materials will have the largest effect. Metallic items (such as the platform) may give a 2% change in count rate when in the near vicinity of the fissile material.

e. Does the real object have moisture, plastic, paper, etc., mixed with the fissile material that was omitted from the MCNP input file? Anything hydrogenous will increase the count rate.

f. A neutron absorber (cadmium, boron) mixed with the fissile material should be included in the material specification. If there is no hydrogenous material, an absorber will not have much effect. But the combination of hydrogenous (moderating) and absorber materials will greatly reduce the fissile rate and the delayed neutron count rate.

g. If the fissile material is a powder, the density of the powder may not be well known. A lower density (and a larger fill height to give the correct mass) will give a slightly larger count rate because there is less self-shielding. A higher density will give a slightly smaller count rate. Even the density of metals is affected by microcracking, although the range of densities is smaller than with powders.

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